



Bioaccumulation Model Calibration Update

March 28, 2018

Overview of Topics

- Status
- Use of CFT algae/phytoplankton data
- Calibration update
 - Overview of process
 - Calibration targets
 - Initial calibration work
- Next Steps

Algae/Phytoplankton from CFT model

- CFT model provides “Concentration in algal particulates” in ng/g of carbon
- Bioaccumulation model needs wet weight concentration (i.e., ng/g ww)
- Equation to convert:

$$C_{ww} = C_{carbon} \times (F_{lipid} + F_{NLOC})$$

Where:

C_{ww} = chemical concentration in wet weight

C_{carbon} = carbon-normalized chemical concentration

F_{lipid} = fraction of lipid in plankton/algae (0.0012)

F_{NLOC} = fraction of NLOC in plankton/algae (0.0388)

Algae/Phytoplankton from CFT model

- Comparison of predicted concentrations for phytoplankton/algae:

Chemical	Model	Phytoplankton Concentrations		
		RM 0-6	RM 6-14.7	RM 14.7-Dam
2378-TCDD	FWM	0.005	0.003	0.00007
	CFT	0.035	0.015	0.00043
TetraCB	FWM	1.9	1.8	1.4
	CFT	41	33	25

- Model impacts:
 - Relatively large increase to phytoplankton (and zooplankton).
 - But minimal impact overall.

Calibration Process

- Evaluate uncalibrated results
- Qualitatively prioritize calibration targets
 - Species
 - Modeling areas
- Sensitivity analysis (to identify key parameters)
- Step-wise calibration for parameters
 - Start with most sensitive assumptions and those that impact all species
 - Identify decision points that may lead to alternate calibrations.
 - Continue refining parameter values.

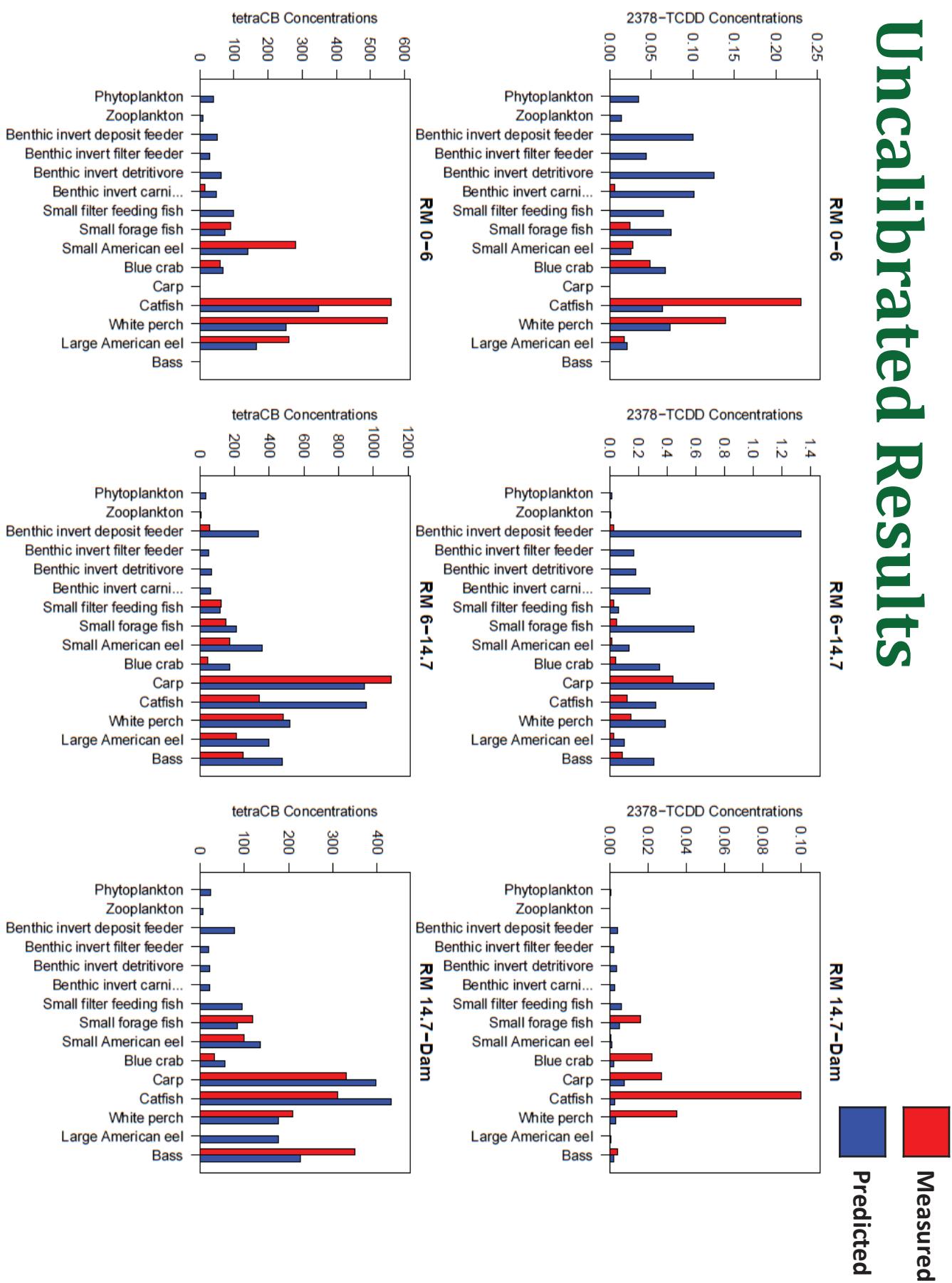
Calibration Targets

- Predictions relative to empirical tissue data:

Model Compartment	Count of Tissue Samples		
	RM 0 – 6	RM 6 – 14.7	RM 14.7 – 17.4
Benthic invertebrate DEPs	-	13	1
Benthic invertebrate C/Os	5	-	-
Small filter feeding fish	-	3	-
Small forage fish	11	13	1
Small American eel (< 50 cm)	3	6	5
Blue crab	19	21	4
Carp	na	11	3
Catfish	6	27	12
White perch	9	8	3
Large American eel (> 50 cm)	3	6	-
Bass	na	4	2

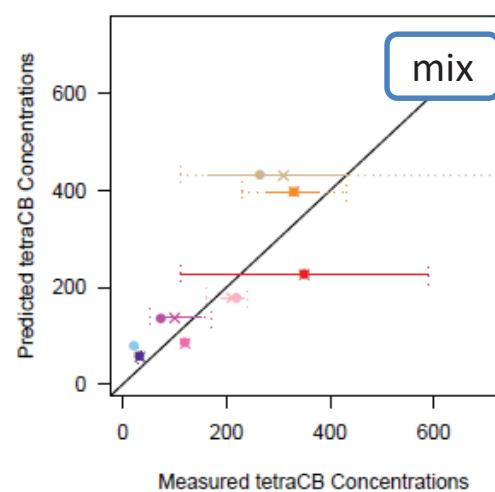
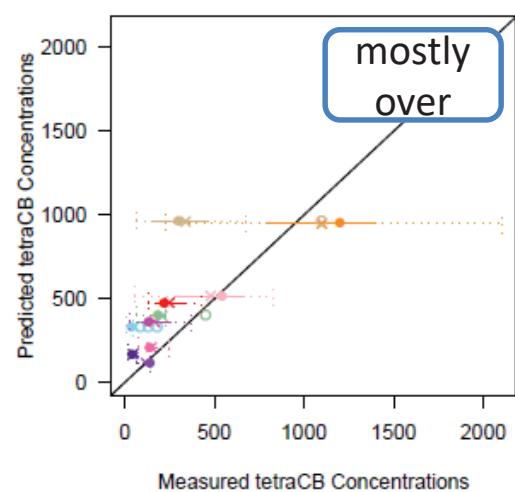
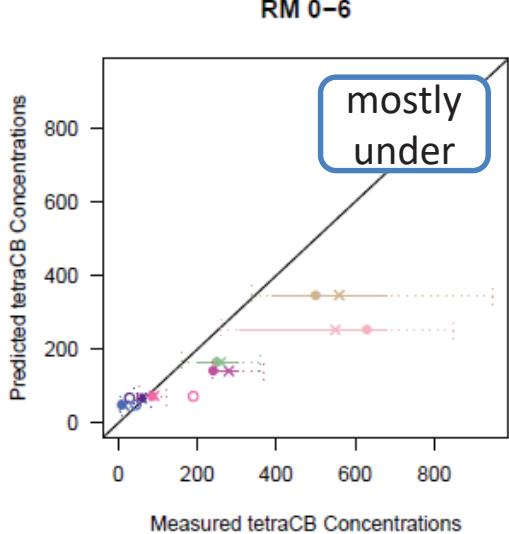
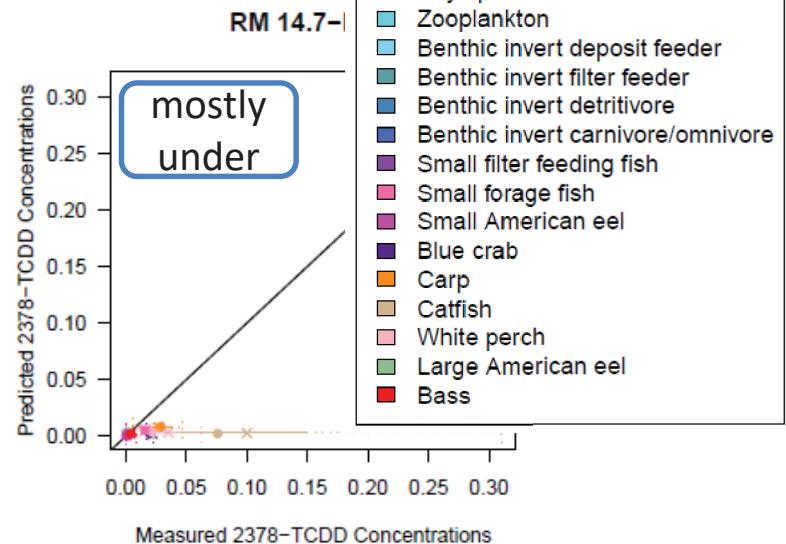
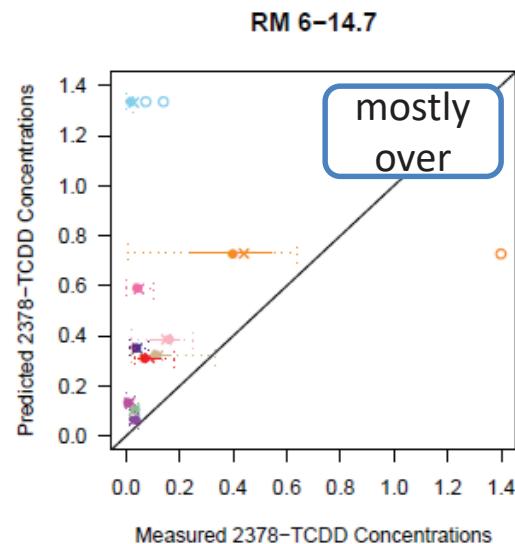
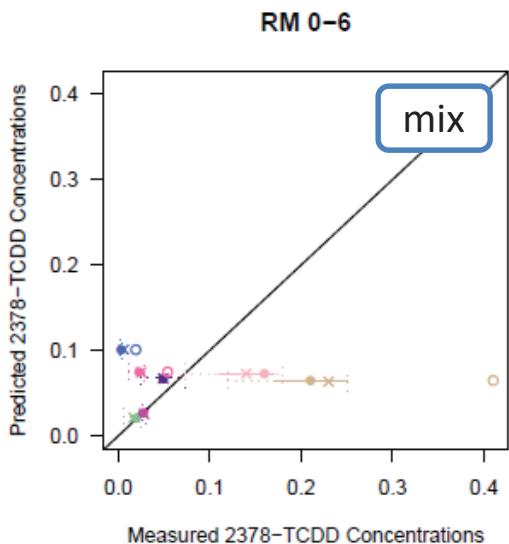
- Predictions for individual samples (select species)
- Will also look at predictions for invertebrates relative to literature BSAFs (per EPA comments)

Uncalibrated Results



Uncalibrated Results

- × Average (Entered in input file)
- Outlier
- Median
- Measured range (25%–75% – boxlot's "box")
- Measured range (boxplot's "whiskers")



Percent Contribution - TetraCB

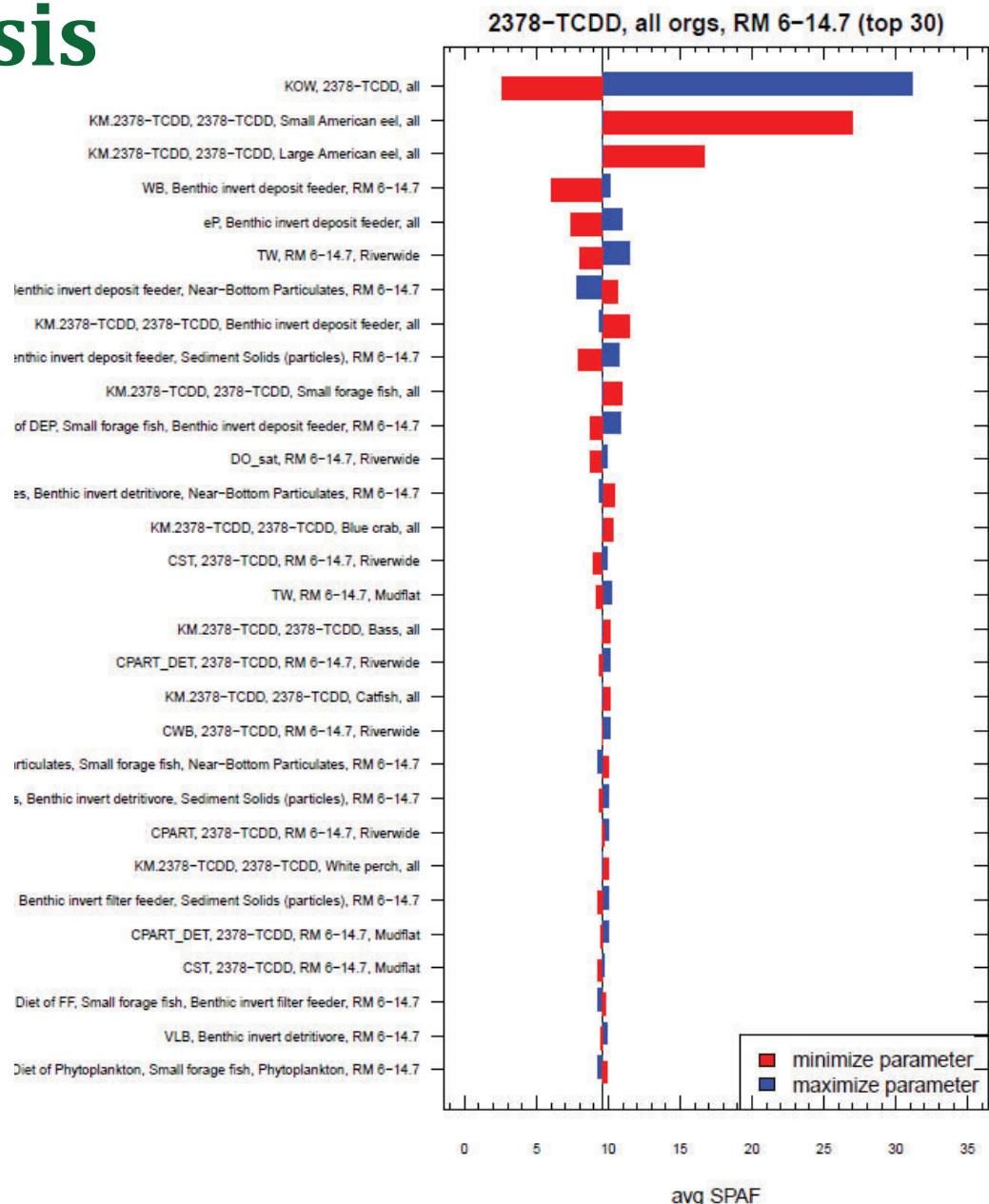
Species Compartment	RM 0 - RM 6					RM 6 - RM 14.7					RM 14.7 - RM 17.4				
	Sediment	Detrital Particulates	Bioavailable Water & Plankton	Porewater	Fluff Layer (NB particulates)	Sediment	Detrital Particulates	Bioavailable Water & Plankton	Porewater	Fluff Layer (NB particulates)	Sediment	Detrital Particulates	Bioavailable Water & Plankton	Porewater	Fluff Layer (NB particulates)
Phytoplankton	0%	0%	100%	0%	0%	0%	0%	100%	0%	0%	0%	0%	100%	0%	0%
Zooplankton	0%	0%	100%	0%	0%	0%	0%	100%	0%	0%	0%	0%	100%	0%	0%
DEP	37%	0%	18%	2%	43%	92%	0%	3%	2%	3%	62%	0%	9%	3%	26%
FF	17%	0%	83%	0%	0%	57%	0%	20%	0%	22%	17%	0%	37%	0%	47%
DET	36%	0%	12%	0%	51%	33%	0%	10%	2%	55%	7%	0%	16%	1%	76%
C/O	22%	0%	26%	3%	48%	48%	0%	13%	11%	28%	18%	0%	25%	8%	50%
Small filter feeding fish	0%	77%	23%	0%	0%	0%	85%	15%	0%	0%	0%	86%	14%	0%	0%
Small forage fish	20%	0%	31%	2%	47%	58%	0%	11%	5%	27%	11%	0%	25%	2%	63%
Small American eel	32%	5%	26%	1%	37%	69%	1%	8%	2%	19%	36%	0%	20%	2%	42%
Blue crab	31%	7%	26%	2%	33%	69%	2%	8%	4%	17%	38%	0%	20%	4%	38%
Carp						67%	0%	4%	2%	27%	28%	0%	9%	1%	62%
Catfish	26%	15%	22%	1%	36%	60%	4%	8%	3%	24%	28%	0%	18%	2%	52%
White perch	23%	8%	28%	1%	40%	63%	2%	10%	3%	22%	32%	0%	21%	2%	45%
Large American eel	23%	16%	26%	1%	34%	59%	5%	10%	3%	22%	29%	0%	21%	2%	47%
Bass						53%	9%	12%	4%	22%	26%	0%	24%	2%	48%

Percent Contribution - 2,3,7,8-TCDD

Species Compartment	RM 0 - RM 6					RM 6 - RM 14.7					RM 14.7 - RM 17.4				
	Sediment	Detrital Particulates	Bioavailable Water & Plankton	Porewater	Fluff Layer (NB particulates)	Sediment	Detrital Particulates	Bioavailable Water & Plankton	Porewater	Fluff Layer (NB particulates)	Sediment	Detrital Particulates	Bioavailable Water & Plankton	Porewater	Fluff Layer (NB particulates)
Phytoplankton	0%	0%	100%	0%	0%	0%	0%	100%	0%	0%	0%	0%	100%	0%	0%
Zooplankton	0%	0%	100%	0%	0%	0%	0%	100%	0%	0%	0%	0%	100%	0%	0%
DEP	55%	0%	9%	1%	35%	98%	0%	0%	1%	1%	37%	0%	2%	1%	61%
FF	35%	0%	65%	0%	0%	85%	0%	4%	0%	11%	8%	0%	9%	0%	83%
DET	53%	0%	4%	0%	42%	64%	0%	2%	1%	33%	2%	0%	2%	0%	96%
C/O	42%	0%	12%	2%	44%	81%	0%	1%	5%	13%	9%	0%	4%	1%	86%
Small filter feeding fish	0%	81%	19%	0%	0%	0%	92%	8%	0%	0%	0%	97%	3%	0%	0%
Small forage fish	35%	0%	20%	1%	44%	88%	0%	1%	2%	9%	11%	0%	4%	1%	85%
Small American eel	51%	2%	14%	1%	33%	90%	0%	1%	1%	8%	18%	0%	4%	0%	78%
Blue crab	51%	3%	14%	1%	31%	90%	0%	1%	2%	7%	19%	0%	4%	1%	76%
Carp						88%	0%	1%	1%	10%	11%	0%	2%	0%	87%
Catfish	45%	9%	13%	1%	34%	87%	1%	1%	2%	9%	13%	0%	3%	0%	84%
White perch	44%	4%	16%	1%	36%	88%	0%	1%	1%	9%	15%	0%	4%	0%	80%
Large American eel	42%	9%	15%	1%	34%	87%	1%	1%	2%	9%	14%	0%	4%	1%	82%
Bass						86%	2%	1%	2%	8%	13%	0%	4%	1%	82%

Sensitivity Analysis

- Objectives:
 - Evaluate model sensitivity to parameters
 - Identify subset of parameters for calibration

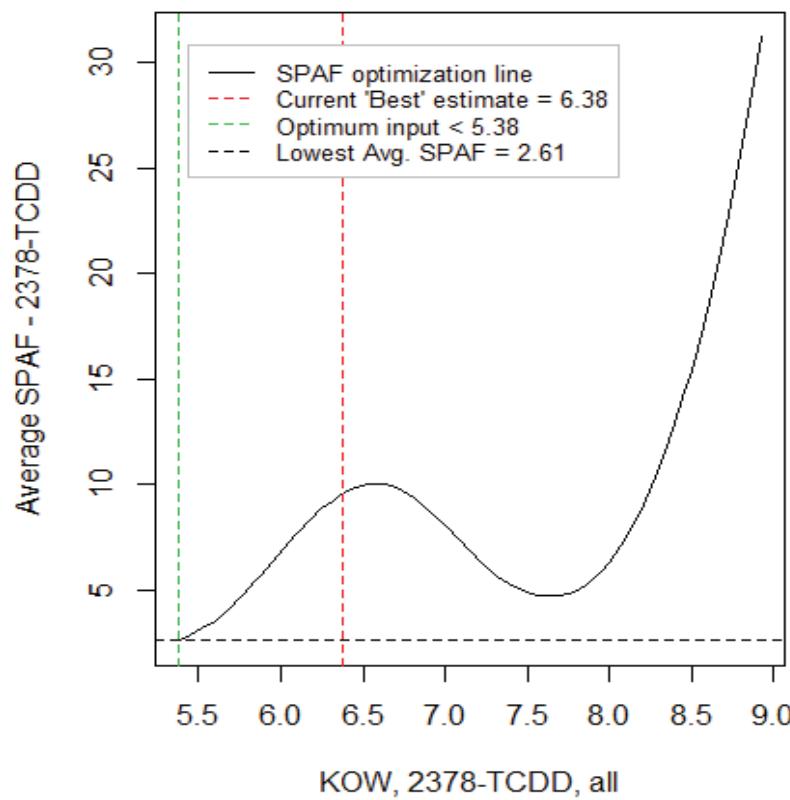


Optimization: K_{OW}

2,3,7,8-TCDD

$$K_{OW} = 6.38 \text{ (5.38 to 8.93)}$$

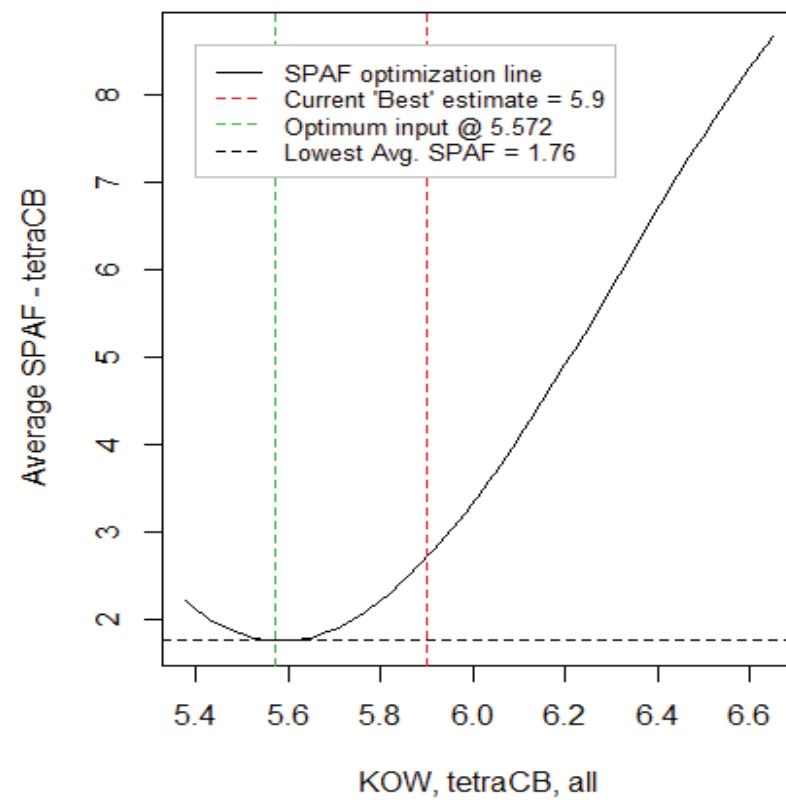
Optimized for all organisms, RM 6-14.7, 2378-TCDD



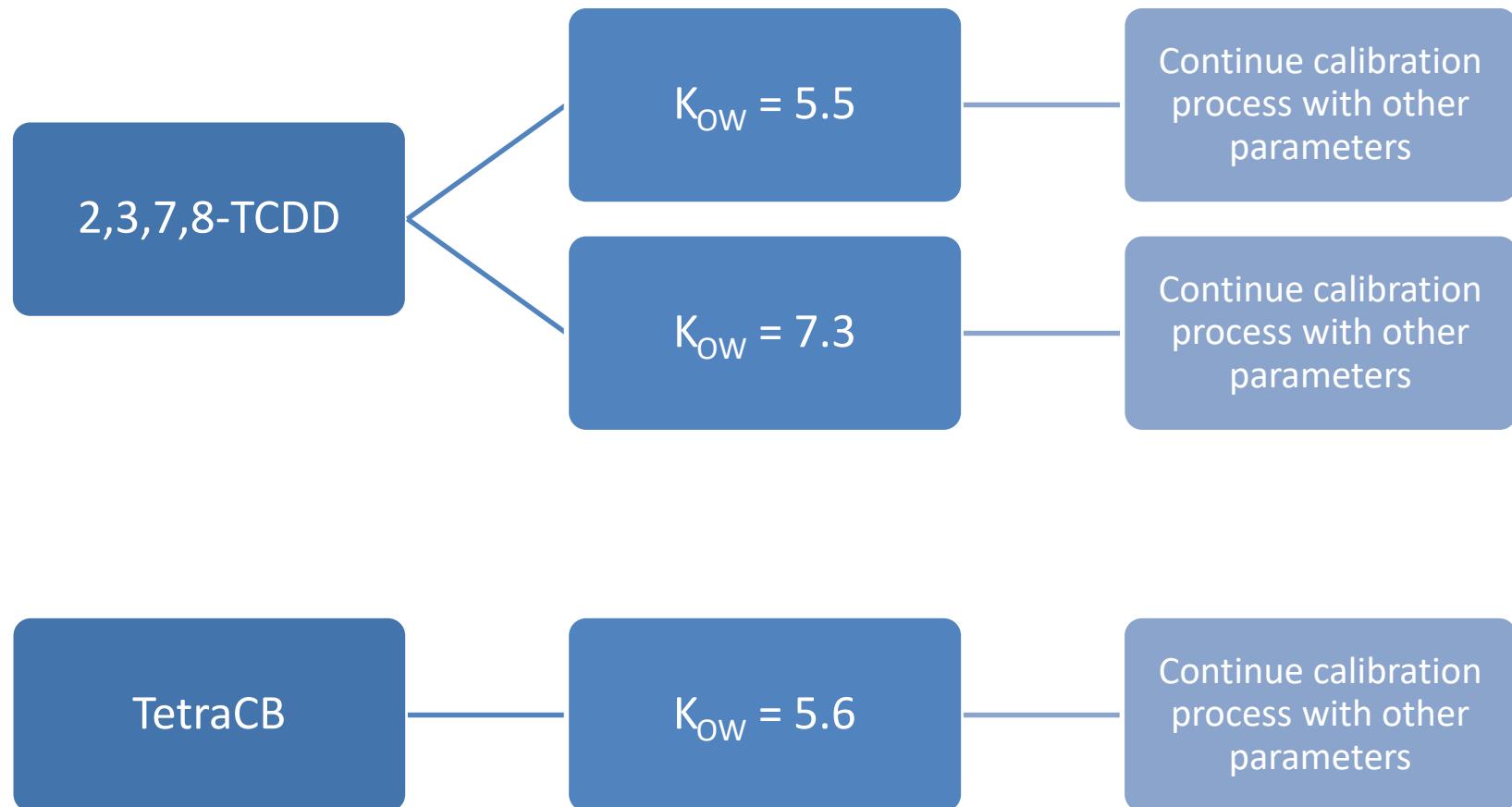
TetraCB

$$K_{OW} = 5.85 \text{ (5.38 to 6.65)}$$

Optimized for all organisms, RM 6-14.7, tetraCB



Calibration Flow Chart: Identification of alternate calibrations



TetraCB: Impact of modifying K_{ow}

Species Compartment	TetraCB					
	Kow = 5.85			Kow = 5.6		
	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder		6.0			3.7	
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omnivore	3.2			1.7		
Small filter feeding fish		-1.0			-1.4	
Small forage fish	-1.2	1.4	-1.4	-2.3	-1.4	-2.5
Small American eel	-2.0	2.1	1.4	-3.4	1.2	-1.3
Blue crab	1.1	3.6	1.7	-1.7	1.8	-1.2
Carp		-1.2	1.2		-1.6	-1.2
Catfish	-1.6	2.8	1.4	-2.9	1.5	-1.4
White perch	-2.2	1.1	-1.2	-4.5	-2.1	-2.5
Large American eel	-1.6	1.9		-2.7	1.0	
Bass		1.9	-1.5		-1.3	-3.6
Average (excluding invertebrates)	1.6	1.9	1.4	2.9	1.5	2.0

TetraCB: Additional modifications (focusing on RM 6-14.7)

Species Compartments	TetraCB			
	Kow = 5.85	Kow = 5.6	Kow = 5.6 minimize % sediment in DEP diet	Kow = 5.6 and minimize weight of DEPs
	no changes	no changes		
Phytoplankton				
Zooplankton				
Benthic invert deposit feeder	6.0	3.7	3.1	1.2
Benthic invert filter feeder				
Benthic invert detritivore				
Benthic invert carnivore/omnivore				
Small filter feeding fish	-1.0	-1.4	-1.4	-1.4
Small forage fish	1.4	-1.4	-1.5	-1.9
Small American eel	2.1	1.2	1.1	-1.3
Blue crab	3.6	1.8	1.6	1.2
Carp	-1.2	-1.6	-1.7	-1.8
Catfish	2.8	1.5	1.4	1.2
White perch	1.1	-2.1	-2.3	-3.2
Large American eel	1.9	1.0	-1.0	-1.2
Bass	1.9	-1.3	-1.4	-1.7
Average (excluding invertebrates)	1.9	1.5	1.5	1.7

2,3,7,8-TCDD: Impact of modifying K_{ow}

Species Compartment	2378-TCDD								
	Kow = 6.38			Kow = 5.5			Kow = 7.3		
	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton									
Zooplankton									
Benthic invert deposit feeder		46			13			36	
Benthic invert filter feeder									
Benthic invert detritivore									
Benthic invert carnivore/omnivore	17			2.9			15		
Small filter feeding fish		2.1			1.3			1.2	
Small forage fish	3.0	12	-3.2	-1.2	2.5	-7.6	1.6	5.4	-7.2
Small American eel	-1.1	10	1.8	-2.4	3.9	-1.2	-3.2	3.0	-1.9
Blue crab	1.4	8.3	-11	-2.7	1.9	-41	-1.7	3.1	-27
Carp		1.7	-3.5		1.1	-4.3		-1.6	-9.3
Catfish	-3.6	2.7	-37	-6.2	1.2	-55	-11.3	-1.4	-130
White perch	-1.9	2.6	-11	-5.4	-1.5	-28	-5.4	-1.3	-33
Large American eel	1.3	3.4		-1.7	1.2		-2.7	-1.1	
Bass		3.5	-1.9		-1.3	-5.1		-1.4	-8.8
Average (excluding invertebrates)	2.0	5.2	10	3.3	1.8	20	4.3	2.2	31

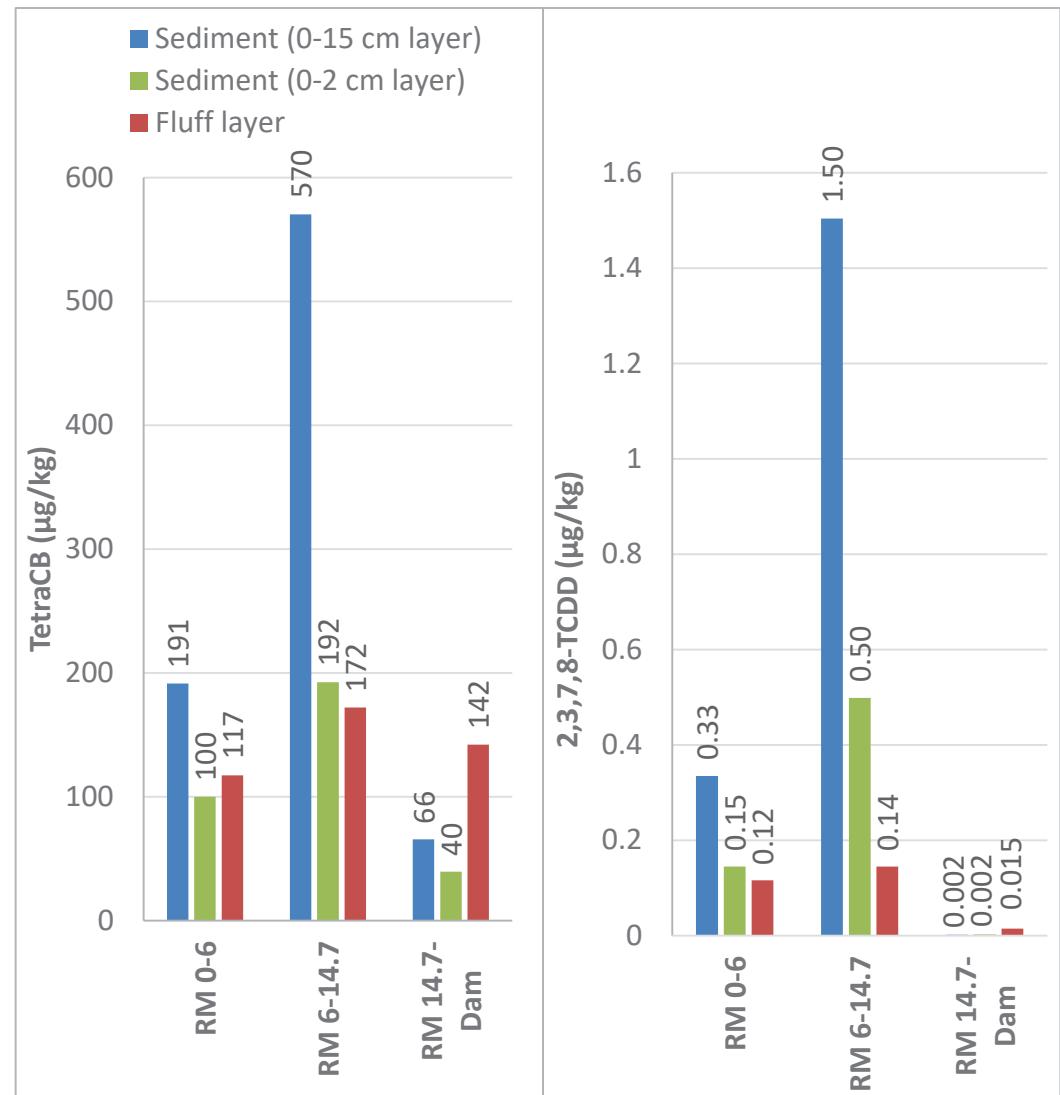
2,3,7,8-TCDD: Additional modifications

(focusing on RM 6-14.7)

Species Compartment	2,3,7,8-TCDD						
	Kow = 6.38	Kow = 5.5			Kow = 7.3		
	-	-	minimize % sediment in DEP diet	and minimize weight of DEPs	-	minimize % sediment in DEP diet	and minimize weight of DEPs
Phytoplankton							
Zooplankton							
Benthic invert deposit feeder	46	13.3	10.4	3.8	36	28	30
Benthic invert filter feeder							
Benthic invert detritivore							
Benthic invert carnivore/omnivore							
Small filter feeding fish	2.1	1.3	1.3	1.3	1.2	1.2	1.2
Small forage fish	12	2.5	2.2	1.6	5.4	4.7	4.8
Small American eel	10	3.9	3.4	2.3	3.0	2.6	2.7
Blue crab	8.3	1.9	1.7	1.2	3.1	2.7	2.8
Carp	1.7	1.1	1.0	-1.0	-1.6	-1.7	-1.7
Catfish	2.7	1.2	1.1	-1.1	-1.4	-1.5	-1.5
White perch	2.6	-1.5	-1.7	-2.8	-1.3	-1.5	-1.4
Large American eel	3.4	1.2	1.1	-1.2	-1.1	-1.3	-1.2
Bass	3.5	-1.3	-1.5	-2.1	-1.4	-1.6	-1.5
Average (excluding invertebrates)	5.2	1.8	1.7	1.6	2.2	2.1	2.1

Impact of inputs from CFT model

- Evaluated range of input values as part of sensitivity analysis
- Further consideration of inputs that are primarily driving the model.
 - 0-15 cm sediment (as compared with 0-2 cm)
 - Fluff layer
- Sediment driving over-prediction issues, especially in RM 6-14.7 modeling area.



Sediment Inputs

- Sediment concentrations
 - Large difference in 0-2 cm vs. 0-15 cm concentrations, particularly for RM 6-14.7.
 - Appears to be adversely impacting calibration
- Possible solution: Consider incorporation of depth weighting factors into model calibration.

Depth Horizon	Sediment Depth-Weighting Factors by Modeling Area		
	RM 0 to 6	RM 6 to 14	RM 14 to 17.4
0 – 2 cm	70% (39 – 95%)	69% (39 – 99%)	99%
2 – 5 cm	12% (12 – 33%)	17% (1 – 33%)	1%
5 – 10 cm	11% (1 – 28%)	14% (< 1 – 28%)	0% (< 1%)
> 10 cm	7% (< 1 – 18%)	0% (< 1%)	0% (< 1%)

TetraCB: Impact of Using Weighted Sediment Concentration

Species Compartment	TetraCB								
	Kow = 5.85			Kow = 5.85			Kow = 5.6		
	sed = 0-15 cm			sed = weighted			sed = weighted		
	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton									
Zooplankton									
Benthic invert deposit feeder		6.0			2.6			1.6	
Benthic invert filter feeder									
Benthic invert detritivore									
Benthic invert carnivore/omnivore	3.2			2.9			1.6		
Small filter feeding fish		-1.0			-1.0			-1.4	
Small forage fish	-1.2	1.4	-1.4	-1.3	-1.1	-1.4	-2.5	-2.0	-2.5
Small American eel	-2.0	2.1	1.4	-2.3	1.2	1.2	-3.9	-1.5	-1.5
Blue crab	1.1	3.6	1.7	-1.0	2.1	1.5	-1.9	1.0	-1.4
Carp		-1.2	1.2		-2.0	1.1		-2.7	-1.3
Catfish	-1.6	2.8	1.4	-1.8	1.8	1.3	-3.3	-1.0	-1.5
White perch	-2.2	1.1	-1.2	-2.4	-1.5	-1.3	-4.9	-3.2	-2.8
Large American eel	-1.6	1.9		-1.7	1.2		-3.0	-1.4	
Bass		1.9	-1.5		1.3	-1.7		-1.8	-4.0
Average (excluding invertebrates)	1.6	1.9	1.4	1.8	1.5	1.3	3.2	1.8	2.1

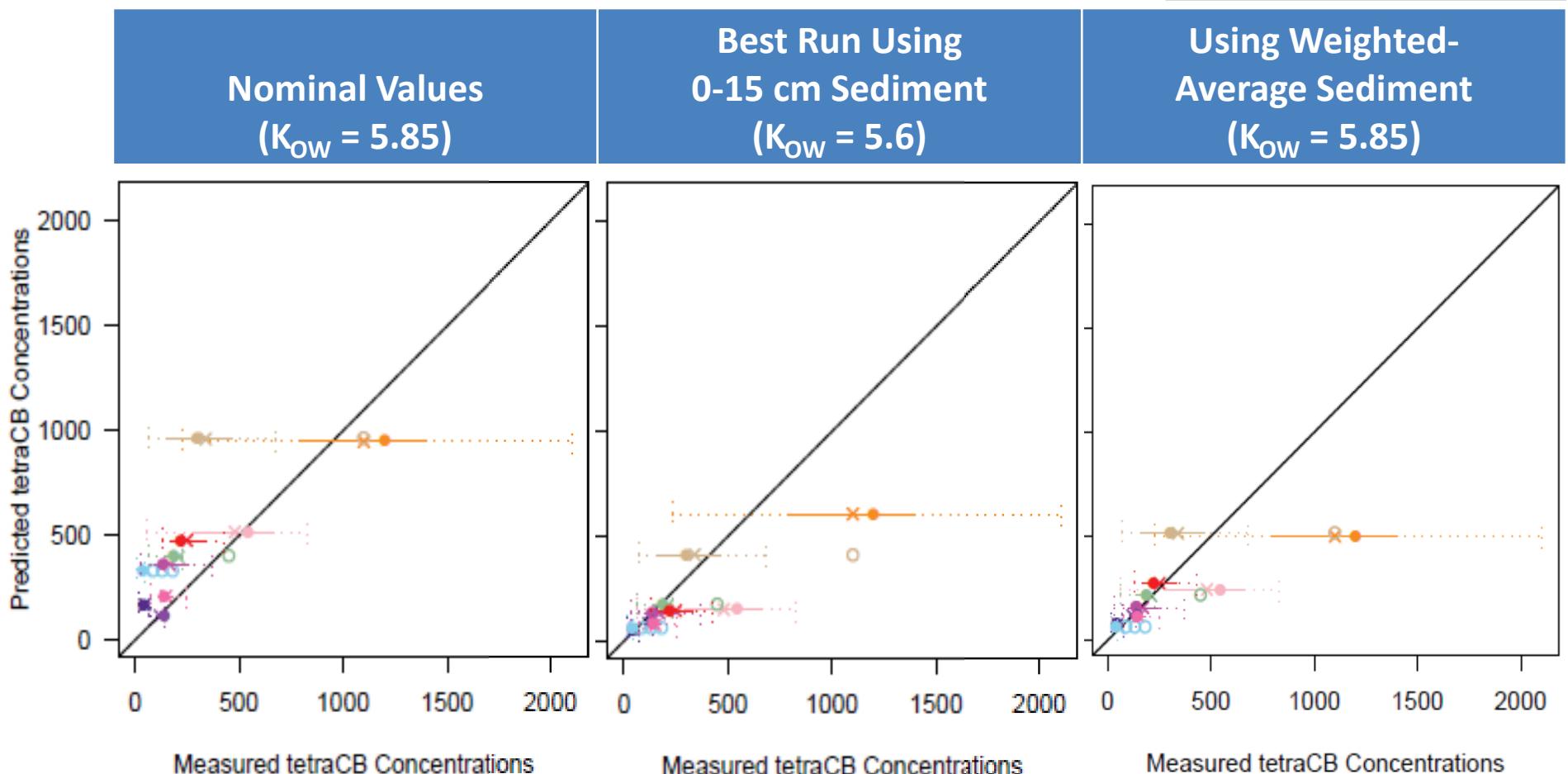
2,3,7,8-TCDD: Impact of Using Weighted Sediment Concentration

Species Compartment	2378-TCDD											
	Kow = 6.38			Kow = 6.38			Kow = 5.5			Kow = 7.3		
	no changes		sed = weighted	sed = weighted		sed = weighted	sed = weighted		sed = weighted	sed = weighted		sed = weighted
	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton												
Zooplankton												
Benthic invert deposit feeder		46			19			5			15	
Benthic invert filter feeder												
Benthic invert detritivore												
Benthic invert carnivore/omnivore	17			13.1			2			13		
Small filter feeding fish		2.1			2.1			1.3			1.2	
Small forage fish	3.0	12	-3.2	2.6	5.5	-2.8	-1.3	1.3	-7.1	1.4	2.7	-6.6
Small American eel	-1.1	10	1.8	-1.4	4.6	2.5	-3.3	1.8	1.1	-4.1	1.5	-1.4
Blue crab	1.4	8.3	-11	1.0	3.8	-7	-3.7	-1.1	-28	-2.2	1.5	-20
Carp		1.7	-3.5		-1.3	-2.8		-1.9	-3.6		-3.3	-7.6
Catfish	-3.6	2.7	-37	-4.6	1.2	-29	-8.0	-1.7	-46	-14.3	-2.8	-106
White perch	-1.9	2.6	-11	-2.4	1.2	-8	-6.5	-2.9	-22	-6.6	-2.5	-26
Large American eel	1.3	3.4		-1.0	1.6		-2.1	-1.7		-3.3	-2.2	
Bass		3.5	-1.9		1.7	-1.5		-2.5	-4.4		-2.6	-7.5
Average (excluding invertebrates)	2.0	5.2	10	2.2	2.6	8	4.2	1.8	16	5	2	25

TetraCB:

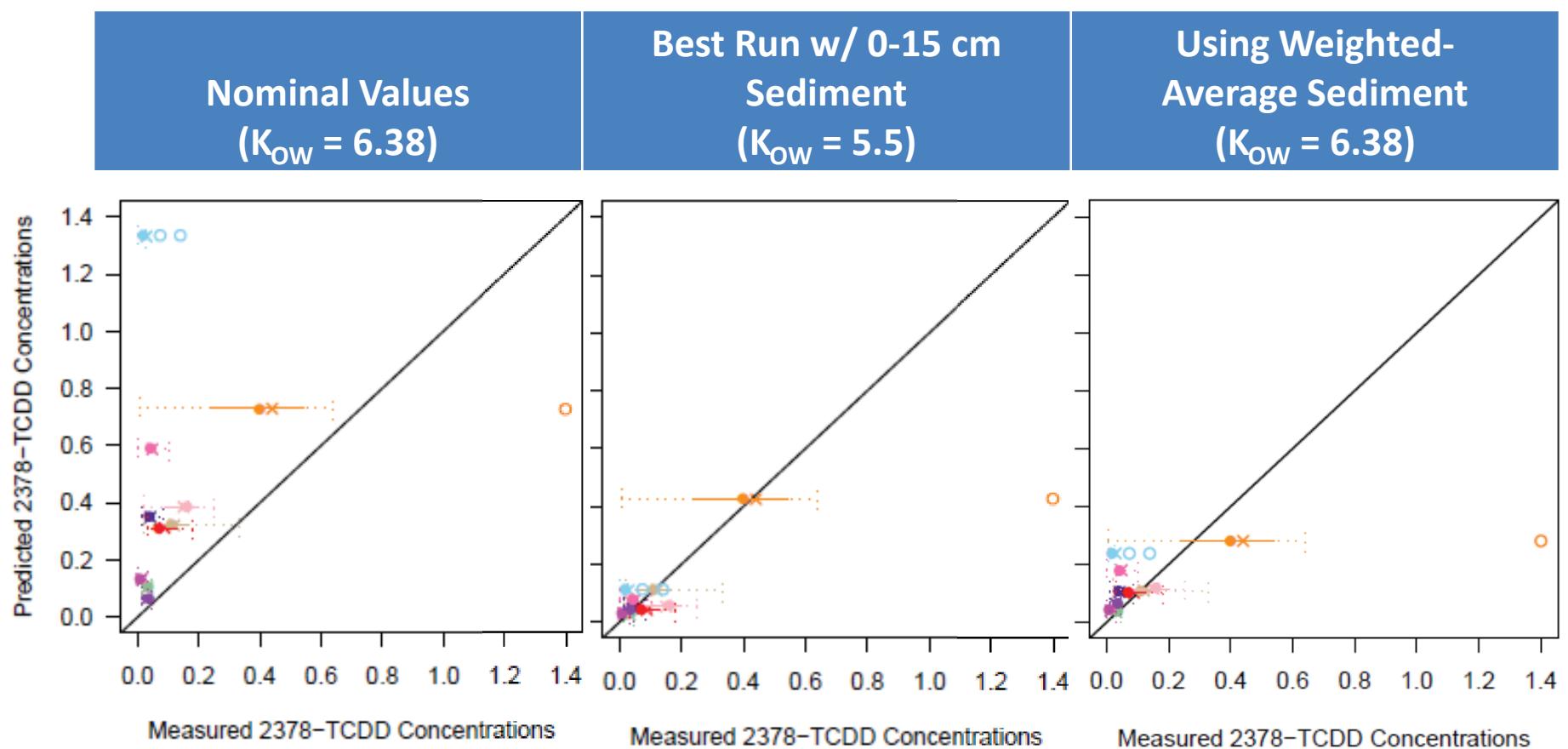
Comparison across runs for RM 6-14.7

- Benthic invert deposit feeder
- Benthic invert filter feeder
- Benthic invert detritivore
- Benthic invert carnivore/omnivore
- Small filter feeding fish
- Small forage fish
- Small American eel
- Blue crab
- Carp
- Catfish
- White perch
- Large American eel
- Bass



2,3,7,8-TCDD: Comparison across runs for RM 6-14.7

- Benthic invert deposit feeder
- Benthic invert filter feeder
- Benthic invert detritivore
- Benthic invert carnivore/omnivore
- Small filter feeding fish
- Small forage fish
- Small American eel
- Blue crab
- Carp
- Catfish
- White perch
- Large American eel
- Bass



Next Steps

- Continue working on calibration using March 21 CFT inputs (or update if needed)
 - Incorporate dynamic model
 - Conduct sensitivity analysis
 - Refining calibration
- EPA feedback?
 - Acceptability of considering depth-weighted sediment concentrations?
 - Other?
- Other topics?